

FY05 LDRD Final Report Coupled Turbulence/Transport Model for Edge Plasmas

T.D. Rognlien, R.H. Cohen, L.L. LoDestro, R.L. Palasek, M.V. Umansky, X.Q. Xu February 9, 2006

LDRD Project Tracking Code: 03-ERD-009

Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

Auspices Statement

This work was performed under the auspices of the U. S. Department of Energy (DOE) by the University of California, Lawrence Livermore National Laboratory (LLNL) under Contract No. W-7405-Eng-48. The project (03-ERD-009) was funded by the Laboratory Directed Research and Development Program at LLNL.

FY05 LDRD Final Report Coupled Turbulence/Transport Model for Edge-Plasmas LDRD Project Tracking Code: 03-ERD-009

Thomas D. Rognlien, Principal Investigator; R.H. Cohen, L.L. LoDestro, R.L. Palasek, M.V. Umansky, and X.Q. Xu, Co-PIs

Abstract

An edge-plasma simulation for tokamak fusion devices is developed that couples 3D turbulence and 2D transport, including detailed sources and sinks, to determine self-consistent steady-state plasma profiles. Relaxed iterative coupling is shown to be effective when edge turbulence is partially suppressed, for example, by shear ExB shear flow as occurs during the favorable H-mode region. Unsuppressed turbulence is found to lead to large, intermittent edge transport events where the coupling procedure can lead to substantial inaccuracies in describing the true time-averaged plasma behavior.

Introduction

Magnetic-fusion energy (MFE) devices are characterized by disparate-scale phenomena whose interaction is critical to their performance. Perhaps foremost among these is the interaction of plasma turbulence with the macroscopic transport (of heat, density, and angular momentum) they drive. Together, these processes determine the energy confinement, and thus the overall device performance. Separately, they are characterized by several orders of magnitude disparity in the time scales.

The computation of turbulence in MFE devices is, even for fixed plasma profiles, an intellectually and computationally demanding activity, and it is typical to perform such calculations to determine single values of local transport coefficients, which depend on the profiles. These coefficients are then compared with those required in transport codes to produce the given experimental profiles to determine if the simulated turbulence can thus reproduce approximate experimental profiles. This approach has had some (limited) success, especially for the core plasmas of tokamaks (the principal MFE device).

In recent years it has become evident that knowledge of the transport in the edge region of MFE plasmas is crucial, not only for material heat-load issues, but also because it determines the effectiveness of an edge "transport barrier" which is central to the confinement properties of the overall device. The edge-region for a tokamak device is shown in Fig. 1, where the red line on the right figure denotes the magnetic separatrix. Magnetic field lines outside the separatrix are unconfined and strike the vessel wall preferentially on the divertor plates indicated schematically as the horizontal boundary at the bottom of the figure. A radial slice of the edge region near the outer-most midplane position in Fig. 1 is shown in Fig. 2. At the inner boundary of the edge region denoted as the pedestal, the higher plasma temperature that sets the edge temperature "boundary

condition" believe key to high core energy confinement. But, in this region, there is little separation of spatial scales between the turbulence and transport, so the turbulent fluxes can be non-local (i.e. they depend on the global shape of the equilibrium densities, temperatures, etc., not just on local values and gradients). This makes a simple parameterization of turbulence difficult, if not impossible. However, because there still is often a time scale separation in the edge, there is a strong motivation to achieve self-consistency between turbulence and transport through coupled, iterative computations.

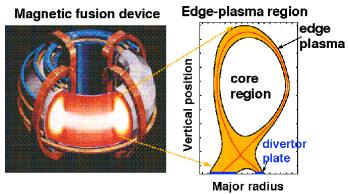


Figure 1. The edge region surrounds the hot core plasma of a tokamak fusion device with a strong confining toroidal magnetic field. The annular edge-plasma region simulated is shown on the right.

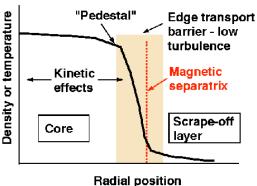


Figure 2. Sharp plasma density and temperature profiles often arise near the magnetic separatrix of a MFE confinement device owing to a transport barrier characterized by low turbulence transport; our modeling will include the so-called pedestal region.

In recent years, LLNL's Fusion Energy Program has played a central role in modeling both edge turbulence with the 3D fluid BOUT code [1,2] and edge transport with the 2D UEDGE code [3,4] used in the national and international MFE community. In addition, we have recently developed some analysis of disparate-scale coupling schemes [5]. The focus of the present work is to demonstrate that it is possible with today's advanced computers to exploit these capabilities by constructing a new model of edge plasma interactions that includes turbulence and transport self-consistently, and thus yield a predictive model for edge plasma characteristics over long device-discharge time scales.

Coupling components and computational infrastructure

In the last 10 years, UEDGE and BOUT, have been developed, refined, and utilized for the study of MFE edge plasmas in the collisional fluid regime. The two-dimensional (2D) UEDGE code assumes toroidal symmetry, and calculates plasma and neutral gas profiles using a set of fluid equations for the density, momentum, and energy of the magnetized plasma and neutrals [3,4]. The neutrals arise from interaction of the edge plasma with material surfaces and from controlled injections. Given a set of empirical radial transport coefficients, which are deduced from experimental data at one location, the plasma parameters throughout the SOL and power deposited on material surfaces are compared to other diagnostics. The commonly good fit lends confidence that, given a set of transport coefficients, the important physical processes are included. A comparison of the experimental and simulated heat flux on the divertor plates (see Fig. 1) of the DIII-D tokamak are shown in Fig. 3 (Ref. 6).

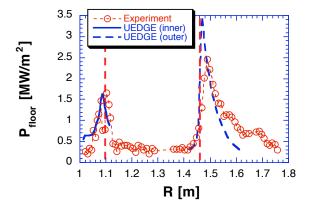


Figure 3. Divertor plate heat-flux profiles calculated by UEDGE compared to DIII-D experimental data; the inner and outer magnetic separatrix strike-points are indicated by vertical red lines.

The 3D BOUT code solves for the saturated spectrum of plasma fluid turbulence and the resulting plasma fluxes for a set of equilibrium edge-plasma profiles [1,2]. There is a different emphasis of the physical processes included in the fluid equations here compared to UEDGE; the inclusion of perpendicular ion inertia and variations in the third toroidal dimension are key to allowing plasma instabilities to develop. The role of turbulence in plasmas is analogous to the behavior found for neutral fluids with large Reynolds number flow where turbulence processes enhance transport far above that from classical collisional processes. For edge plasmas, the turbulence is often driven by the free energy provided by steep gradients in the equilibrium plasma profiles at the edge. The steep gradients are the result of good magnetic confinement in the core region giving way to poor confinement in the scrape-off layer where magnetic field lines have direct contact with material surfaces. The large fluctuation levels observed in the edge compared to the core can be partially understood from the stronger edge-gradient instability drive. The strong turbulence developed in the edge region from BOUT

compares well with experimental measurements of density fluctuations on the DIII-D tokamak as shown in Fig. 4. Here one can see that the size of the turbulent eddies is a few centimeters, the same scale as gradients in edge-plasma parameters. Also note that the turbulence can be strong, with density fluctuation levels of ~50%. Through the LDRD work in FY04 we have substantially improved the diagnostic capability to better understand the correlation between midplane and divertor fluctuations is shown in Fig. 4b [7].

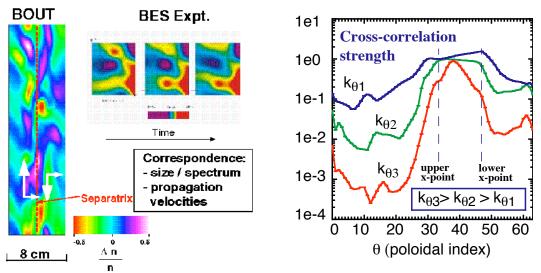


Figure 4. Edge-plasma density fluctuations at the outer midplane as calculated by LLNL's BOUT code compared to beam-emission-spectroscopy (BES) diagnostic on the DIII-D tokamak. Beam Emission Spectroscopy data of density fluctuations shows 3 closely-spaced time frames over a 4x4 cm2 area. On the right, modes with large toroidal wavenumber are shown to be weakly correlated between the midplane and divertors.

UEDGE and BOUT already have several important points of contact in their geometry and models for the full toroidal geometry of tokamaks with magnetic divertors. Both codes describe the plasma using fluid equations and use a common computational mesh based on the magnetic flux surfaces from MHD equilibria for specific core-plasma conditions. Being 3D, BOUT is computationally intensive, taking on the order of 2 days using 64 processors to obtain a well-saturated turbulence spectrum. Both BOUT and UEDGE use implicit methods for efficient time advancement of the equations [8].

Another key aspect of this project is that we have research experience coupling schemes [5]. In that work, we developed algorithms for simultaneously solving the turbulence and transport equations on their separate timescales for simple model problems. The approach was to alternately iterate a solution of the transport equations and time-stepping the turbulence equations, with consistency achieved for the final steady-state solution. This technique was applied to a simple model turbulence/transport system involving a 1D transport solver (which evolves the background density profile only and whose gradient drives the turbulence) and a 2D, two-field turbulence code. Here we were able to achieve self-consistent solutions for steady-state background profiles and statistically steady-state turbulence in a computation time about the same as that required for the turbulence code alone to saturate for a fixed background profile, and

a time much smaller than that required for the turbulence code alone to evolve the background profile to its steady state. Our project will develop extensions and variations of these algorithms as a means of coupling 2D edge transport and 3D edge turbulence that ultimately allows a large time-step implicit advancement of the transport. This is a major challenge, as these systems are substantially more complex than the model problems in Ref. [5].

The plasma fluid equations [for density, parallel (along $\bf B$) velocity, and electron and ion temperatures] can be written in the form as illustrated by the particle continuity equation for the total ion density, N_i + n_i , where N_i is the density averaged toroidally, and n_i contains all of the toroidal variations. For edge plasma microturbulence in tokamaks, n_i generally contains the fast temporal variations as well. The ion continuity equation is thus

$$\partial(N_i + n_i) / \partial t + \nabla \bullet [(N_i + n_i) V_i] = S_p$$
,

where V_i is the ion velocity, and S_p is the particle source from ionization of neutrals. The evolution on N_i is described by UEDGE and the rapidly fluctuating n_i is simulated by BOUT.

Averaging over the toroidal direction, denoted by $\langle \rangle$, yields a transport equation for N_i as used by UEDGE:

$$\partial N_i^m / \partial t + \nabla \bullet (N_i^m V_{\parallel i}^m + \Gamma_r^{m-1}) = \langle S_p \rangle^m,$$

where the superscript m denotes an iteration index for the transport/turbulence coupling. The parallel velocity is dominated by the toroidally averaged velocity V_{li} . The perpendicular or radial particle flux is dominated by microturbulence, and comes from the BOUT simulation:

$$\Gamma_{\rm r}^{\rm m-1} = (1 - a_1) \Gamma_{\rm r}^{\rm m-2} + a_{\rm f} < n_{\rm i} v_{\rm ri} >^{\rm m-1},$$

where a_f is a relaxation parameter, and v_{ri} is the full 3D, rapidly fluctuating radial fluid velocity from BOUT. In adding Γ_r^{m-1} to UEDGE, the flux is divided into an effective diffusion coefficient, D, and a convective velocity, V_N , as follows:

$$\Gamma_{\rm r}^{\rm m-1} = -D \; dN_{\rm i}/dr + V_{\rm N} \; N_{\rm i}. \label{eq:gamma_rate}$$

In the iterative coupling, the ion profile in BOUT is similarly updated according to

$$N_i^{m-1} = (1 - a_p) N_i^{m-2} + a_0 N_i^{m-1},$$

where a_p is a second relaxation parameter.

This overall iteration procedure is know as Relaxed Iterative Coupling (RIC), and its stability properties are analyzed for some simple systems in Ref. [5]. Here we are applying the procedure to a more complicated equation set that includes multiple variables with cross-coupling. In the application below, we couple density, electron temperature, and ion temperature, with the partial coupling to the parallel velocity as

well. This coupling scheme can be effective when there is a significant time scale separation between the evolution of N_i and the turbulence fields as represented by n_i (or similarly, the potential ϕ). In Fig. 5, we show typical time scales from DIII-D simulations for N_i from UEDGE and ϕ from BOUT, indicating approximately two orders of magnitude time scale separation.

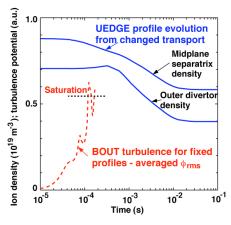


Figure 5. Evolution of the toroidally averaged edge-plasma density from UEDGE and the 3D fluctuating potential from BOUT for the DIII-D tokamak showing a time scale separation of approximately two orders of magnitude.

Application of the coupling method to edge-plasma geometries

The RIC scheme has been applied to both the DIII-D single-null divertor geometry with X-point and full particle divertor recycling within UEDGE and a circular limiter geometry. These two geometries are shown in Fig. 6.

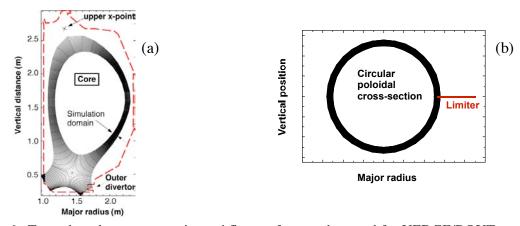


Figure 6. Two edge-plasma geometries and flux-surface meshes used for UEDGE/BOUT coupling: (a) DIII-D single-null and (b) a limiter configuration.

Divertor geometry

The turbulence simulations with BOUT in the divertor geometry are more demanding in terms of time step and this has been identified as due to the large shear in the magnetic field near the X-point. For an initial demonstration, we show results for

coupling only the density variable for fixed energy transport coefficients (χ_e , χ_i) and perpendicular parallel viscosity (η), with a limited number of iteration owing to the large computer time needed for the turbulence simulations. Such results are shown in Fig. 7 for the effective density diffusion coefficient, D [9].

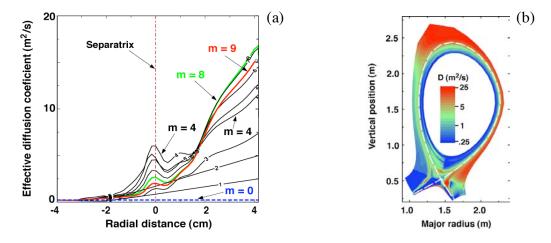


Figure 7. Iteration history of density diffusion coefficient (D) at (a) the outer midplane, and (b) the poloidal distribution of D for the final iteration m=9 over for UEDGE/BOUT coupling for a single-null DIII-D geometry.

Coupled simulations for the divertor geometry has been extended to coupling the ion and electron temperatures as well via BOUT-determined transport coefficients $\chi_{e,I}$ [10]. In addition, this coupling example characterized the radial transport as 50% diffusion and 50% convection. The correspond convective velocities for density and temperatures are shown in Fig. 7. Such a separation between diffusion and convection allows the modeling of transport that can be in a direction "up" the density gradient, which can occur in BOUT simulations. As long as the total flux is correct, the division between a spatially dependent diffusion and convective velocities do not matter to the transport calculation. Of course, the physical picture of the rapidly increasing D and/or V_N is consistent with the notion of plasma blob propagation [krash].

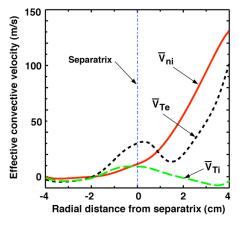


Figure 7. Convective transport velocities for DIII-D single-null case with 50/50 split of turbulent transport between convection and diffusion.

Limiter geometry

For the limiter geometry in Fig. 6b, BOUT has approximately an order of magnitude increase in the time step, which allows more detailed assessment of the convergence properties of the coupling strategy.

Three cases are considered here to contrast the behavior of the edge and the viability of the coupling for a case with unsuppressed turbulence (case 2), and two cases of suppressed turbulence, one with an adhoc damping term (case 1) and the second with the more realistic stabilization by ExB shear flow (case 3). All case use relaxation coefficients for the fluxes and the profiles (a_f and a_p) are 0.25, and we use a equal division of the fluxes between diffusion and convection. The results for case 1 are shown in Fig. 8 and 9, where the density profile relaxes to a near steady-state after about 15-20 iterations and remains steady.

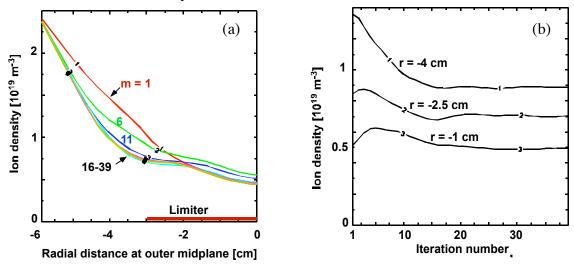


Figure 8. History of outer midplane density over m coupling iterations: (a) density versus radius, and (b), density versus iteration number.

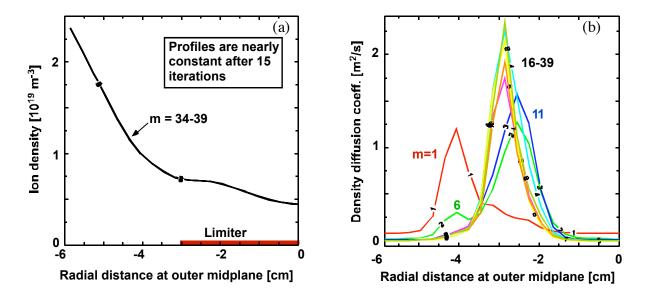


Figure 9. (a), Data for radial profile from Fig. 8a for last 5 iterations, and (b), diffusion coefficient for all iterations.

The second case substantially reduces the damping away from the wall by having it decay strongly away from the boundary. The result on the density and density diffusion coefficient are shown by the brown-shaded region in Fig. 10. Note that the density is far less steady with large excursions produced by the large transport events, especially for r < 0 as seen in Fig. 10b (red and green curves). The oscillations in the density occur even with the 0.25 relaxation factor for both N_i used in the BOUT and D used in UEDGE. There are substantial dynamics associated with these large events that are not captured by the coupling.

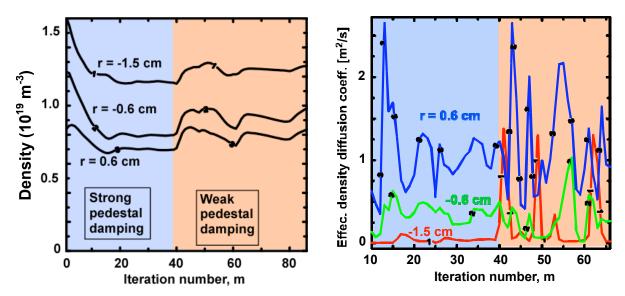


Figure 10. (a), midplane density versus iteration number for strong and weak damping cases, and (b), the associated variation in the diffusion coefficients.

Finally, we consider case 3 with weak damping, but the presence of a radial electric field profile as shown in Fig. 11a corresponding to that expected for H-mode plasmas, but from transport modeling and from experimental measurements. In Fig. 11b, one sees that the density again returns to a near steady-state without the very large oscillations seen in Fig. 10b for m > 39 (weak damping, but no shear flow).

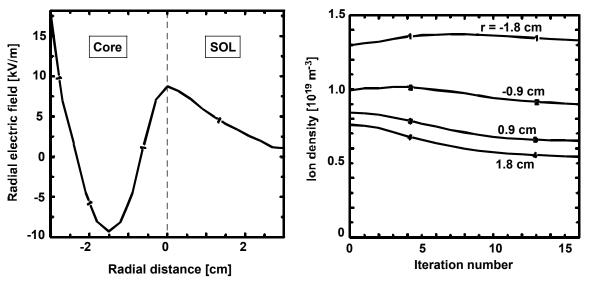


Figure 11. (a), The radial electric field profile to mimic H-mode plasma conditions with ExB flow shear, and (b), the resulting density variation with iteration number showing a return to quasi-steady behavior (compare to weak damping case in Fig. 10a.

The difference in the turbulence spatial characteristics is shown in Fig. 12a for case 2 during a large fluctuation, and in Fig. 12b for case 3. Note that the amplitude of the turbulent δn is a factor of 2.5 lower for the shear flow case (b), and a smaller spatial structure. A time-dependent movie of this fluctuation shows how the shear flow (downward poloidally for r < 0 and upward for r > 0) appears to prevent the large mode in (a) from developing.

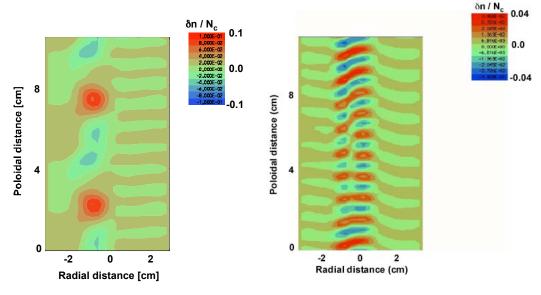


Figure 12. (a), The fluctuating density near the midplane for weak shear during a large event, and (b), the fluctuating density for a case of ExB shear-flow suppression.

Applicability and summary

The results of the edge-plasma coupling LDRD project show the RIC scheme for coupling turbulence and transport for realistic parameters and multiple variables works for situations where the turbulence is partially suppressed. Since the time scale separation between the turbulence saturation and transport is about two orders of magnitude, and ~10 iterations can yield a quasi-steady solution, the coupling provides an order of magnitude improvement over brute-force running of the turbulence simulation evolving its own profile over this same time.

Fortunately, the situation of partial edge-turbulence suppression is just that found in the favorable H-mode regime for tokamaks where it is believed that ExB shear flow provides the suppression. Consequently, the technique has good application to this situation.

This coupling capability was one of the components of our proposal for extended funding from DOE OFES kinetic edge-code development, where this key issue arises. This kinetic edge code development has recently been funded at the 500k level from OFES.

References

- 1. X.Q. Xu, R.H. Cohen, T.D. Rognlien, and J.R. Myra, "L-H transition simulations in divertor geometry," Phys. Plasmas **7** (2000) 1951; X.Q. Xu, W.M. Nevins, T.D. Rognlien *et al.* "Transitions of turbulence in plasma density limits," Phys. Plasmas **10** (2003) 1773.
- X.Q. Xu, R.H. Cohen, W.M. Nevins, G.D. Porter, M.E. Rensink, T.D. Rognlien, J.R. Myra, D.A. D'Ippolito, R. Moyer, P.B. Snyder, and T.N. Carlstrom, "Turbulence simulations of X-point effects on the L-H Transitions," Nucl. Fusion 42 (2002) 21.
- 3. T.D. Rognlien, D.D. Ryutov, N. Mattor, and G.D. Porter, "Two-dimensional electric fields and drifts near the magnetic separatrix in divertor tokamaks," Phys. Plasmas 6 (1999) 1851.
- 4. T.D. Rognlien and M.E. Rensink, "Edge-plasma models and characteristics for magnetic fusion energy devices," Fusion Eng. Design **60** (2002) 497.
- 5. A.I. Shestakov, R.H. Cohen, J.A. Crotinger, L.L. LoDestro, A. Tarditi, and X.Q. Xu, "Self-consistent modeling of turbulence and transport," J. Comp. Phys. **185** (2003) 399.
- G.D. Porter, R. Isler, J. Boedo, and T.D. Rognlien, "Detailed comparison of simulated and measured plasma profiles in the SOL and edge plasma of DIII-D," Phys. Plasmas 7 (2000) 3663.

- 7. M.V. Umansky, T.D. Rognlien, X.Q. Xu, "Simulation of turbulence in the divertor region of tokamak edge plasmas," J. Nucl. Mater., submitted (2004).
- 8. T.D. Rognlien, X.Q. Xu, and A.C. Hindmarsh, "Implementation of parallel implicit methods for edge-plasma numerical simulations," J. Comp. Phys. **175** (2002) 249.
- 9. T.D. Rognlien, M.V. Umansky, X.Q. Xu et al, "Self-consistent simulation of turbulence and transport in tokamak edge plasmas", Contrib. Plasma Phys. **44** (2004) 188.
- 10. T.D. Rognlien, M.V. Umansky, X.Q. Xu et al. J. Nucl. Maters. **337-339** (2005) 327.
- 11. J.A. Boedo, D.L. Rudakov, R.A. Moyer et al., Phys. Plasmas 10 (2003) 1670.
- 12. M. Kotschenreuther, T.D. Rognlien, and P. Valanju, "Implications of convective scrape-off layer transport for fusion reactors," Fusion Eng. Design, submitted (2004).
- 13. T.D. Rognlien, M.V. Umansky, X.Q. Xu et al., "Simulation of plasma fluxes with self-consistent edge turbulence and transport," J. Nucl. Mater., submitted (2004).
- 14. M.V. Umansky, T.D. Rognlien, X.Q. Xu et al, "Turbulence in the divertor region of tokamak edge plasmas," Contrib. Plasma Phys. **44** (2004) 182.
- 15. X.Q. Xu, W.M. Nevins, R.H. Cohen et al. "Correlation of density pedestal width and neutral penetration length," Contrib. Plasma Phys. **44** (2004) 105.